ELSEVIER

Progress in Nuclear Magnetic Resonance Spectroscopy

PROGRESS IN NUCLEAR
MAGNETIC RESONANCE
SPECTROSCOPY

www.elsevier.nl/locate/pnmrs

Author Index, Volume 35

Antzutkin, O. N. 203
Abraham, R. J. 85
Auger, M. 1

Berthault, P. 295

Davis, J. H. 1
Desvaux, H. 295

Fukui, H. 267

Gounarides, J. S. 153

Horsewill, A. J. 359

Shapiro, M. J. 153

Vlahov, G. 341

ELSEVIER

Progress in Nuclear Magnetic Resonance Spectroscopy

PROGRESS IN NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

www.elsevier.nl/locate/pnmrs

Subject Index, Volume 35

Affinity NMR **35** 191–5
Anisotropy
  C-C bond **35** 100–1
  carbonyl **35** 146–9
Anti-TOSS signal **35** 232–3
Atomic charges **35** 86
Automated sample changing **35** 178
Automated spectral analysis **35** 180–1
Autoxidation **35** 345
Axial diffusion **35** 26

B_1 field inhomogeneity **35** 309
Bacterial chemotaxis membrane receptor **35** 77
Bacteriophage coat proteins **35** 17–24
Bacteriorhodopsin (bR) **35** 62–5, 72–6
Bathorhodopsin **35** 67
Bimolecular dynamics **35** 323–9
Biomolecules, steady-state magnetization **35** 333–4
Bipolar pulse longitudinal eddy-current delay (BPP-LED) **35** 188
Bond anisotropy **35** 100–1
BPP-LED . *see* Bipolar pulse longitudinal eddy-current delay
bR . *see* Bacteriorhodopsin
Bromine chemical shifts **35** 121–34

^{13}C
  chemical shifts **35** 155–6
  relaxation **35** 156–8
^{13}C MAS NMR **35** 169–70
^{13}C multiple-quantum excitation **35** 205
^{13}C NMR **35** 342–3
  CSA **35** 13
  gel-phase **35** 161–2
  gramicidin A **35** 29–34
  membranes **35** 4–5
  methyl groups **35** 377
  olive oil **35** 345–56
^{13}C-^{15}N bond vectors **35** 36
C-C bond anisotropy **35** 100–1
Carbonyl anisotropy **35** 146–9
Carbonyl carbon resonance **35** 346
Carbonyl substituent chemical shifts **35** 140–9
Carousel-symmetry **35** 223–4
CC . *see* Coupled-cluster
CCPPA . *see* Coupled-cluster polarization propagator
C...H steric interactions **35** 97–9
Charge effects **35** 86–7
Chemical shift anisotropy (CSA) **35** 4, 12–7, 209–10, 298
  relaxation rates **35** 301–2
  single crystal measurements **35** 250
  static powder pattern **35** 250–1
Chemical shift tensors **35** 260
  direct time-domain calculations **35** 252–5
  Herzfeld and Berger analysis **35** 252
  Maricq and Waugh moment analysis **35** 251–2
^{15}N NMR **35** 30–4
Chemical shifts **35** 209–10
  see also Proton chemical shifts; Substituent chemical shifts
  ^{13}C **35** 155–6
  carbonyl substituent **35** 140–9
  gramicidin A **35** 34–9
  hydrocarbon **35** 95–109
  perturbation method **35** 185–6
  retinal carbons **35** 62–3, 67
CHF . *see* Coupled Hartree-Fock
Chlorine chemical shifts **35** 116–21
Chlorosteroids **35** 116
Combinatorial chemistry **35** 153–200
Coupled Hartree-Fock (CHF) approximation **35** 270–4
Coupled spins **35** 220–1
Coupled-cluster (CC) method **35** 287–93
Coupled-cluster polarization propagator (CCPPA) method **35** 291–2
CP . *see* Cross-polarization
Cross-polarization (CP) **35** 5, 205–6
Cross-relaxation **35** 297, 303–4, 319–21, 328–9
CSA . *see* Chemical shift anisotropy
Cyclohexanes

PII: S0079-6565(00)00030-3

charge effects **35** 87
proton chemical shifts **35** 90, 108

2D NMR **35** 170
2D-PASS **35** 237
DEPT . *see* Distortionless enhancement by polarization transfer
Diffusion, resins **35** 158–9
Diffusion-ordered NMR (DOSY), mixture analysis **35** 190–1
Dipolar coupling **35** 3, 4, 245–8, 262–3
bacteriophages **35** 17
Dipolar interactions **35** 6–11, 298
relaxation rates **35** 301–2
Dipolar recovery at the magic angle (DRAMA) **35** 71
Dipolar splitting **35** 8–11, 36–9
Distortionless enhancement by polarization transfer (DEPT) **35** 349–50
Divinyl benzene (DVB) gel beads **35** 155
DNP . *see* Dynamic nuclear polarisation
DOSY . *see* Diffusion-ordered NMR
Double quantum excitation **35** 205
Double sideband irradiation **35** 374
DRAMA . *see* Dipolar recovery at the magic angle
DVB . *see* Divinyl benzene
Dynamic nuclear polarisation (DNP) **35** 367

Electric fields **35** 109–16
calculation **35** 86
Electric quadrupolar Hamiltonian **35** 4
Electron-nuclear interactions **35** 268
ESR tunnel resonance spectroscopy **35** 367–8
Ethanes, partial atomic charges **35** 91–4
Ethers, oxygen SCS **35** 134–40
Ethyl chloride **35** 116
Euler angles **35** 211–3

^{19}F NMR, gel-phase **35** 162–5
Fast exchange **35** 305–6, 321–3, 325–7
Fd virus **35** 19–21
Filtering **35** 205
Flow-through probes **35** 179
Fluorine substituent chemical shifts **35** 109–16
Free evolution propagator **35** 218

Gel-phase ^{13}C NMR **35** 161–2
Gel-phase ^{19}F NMR **35** 162–5
Gel-phase ^{31}P NMR **35** 165–7
Glycerides **35** 343–4
Glycerol carbon resonances **35** 350–2
Glycophorin A **35** 76
Gradient MAS probe **35** 178
Gramicidin A **35** 24–61, 70–1, 77

^{1}H MAS NMR, resolution **35** 171–2
^{1}H multiple-quantum spectroscopy **35** 205
^{1}H NMR **35** 342–3
membranes **35** 4–5
olive oil **35** 343–5
solvents **35** 167–8
^{1}H spin diffusion **35** 68
^{2}H NMR
gramicidin A **35** 25–8
membranes **35** 4–5
quadrupolar interaction **35** 16–7
Halocyclohexanes **35** 127–31
Halogens, steric coefficients **35** 131–4
Haupt effect **35** 377–9
Heteronuclear dipolar interactions **35** 61
Heteronuclear dipole-dipole interactions **35** 4
Heteronuclear multiple quantum correlation (HMQC) **35** 5
Heteronuclear single quantum correlation (HSQC) **35** 5
H...H steric interactions **35** 95–7
High throughput NMR **35** 178–80
High-field NMR spectrometers **35** 2
High-resolution solid-state NMR
bacteriorhodopsin **35** 62
distance determination **35** 71
High-resolution solution NMR **35** 2
High-speed ^{1}H MAS **35** 68–70
HMQC . *see* Heteronuclear multiple quantum correlation
Homonuclear dipolar interactions **35** 61
Homonuclear spin-spin interaction **35** 210–1
HPLC-NMR **35** 181–5
HSQC . *see* Heteronuclear single quantum correlation
Hydrocarbon chemical shifts **35** 95–109

INEPT . *see* Insensitive nucleus enhancement by polarization transfer
Insensitive nucleus enhancement by polarization transfer (INEPT) **35** 5
Interproton distances **35** 315–7
Intramolecular exchange **35** 318–9
Iodine chemical shifts **35** 121–34
IRS . *see* Isotropic rotation sequences
Isotope effects **35** 385–6
Isotropic chemical shift **35** 209
Isotropic pitch **35** 255
Isotropic rotation sequences (IRS) **35** 207, 255–63

Large molecules **35** 317–8
LED . *see* Longitudinal eddy-current delay
Level-crossing spectroscopy **35** 367
Linear electric fields **35** 86
Linear response function **35** 285–7
Liquids, dynamic processes **35** 295–340
Longitudinal eddy-current delay (LED) **35** 188
Low-field dipole-dipole driven NMR **35** 374–5

Magic angle spinning (MAS) **35** 1–84, 213–5
  multipin crowns **35** 176
  resins **35** 158, 167–78
  single bead analysis **35** 173–6
Magic angle spinning NMR (MAS NMR), sideband manipulation **35** 203–66
Magic-angle-turning (MAT) **35** 260
Magnetization build-up **35** 313–4
Maricq and Waugh moment analysis **35** 251–2
MAS . *see* Magic angle spinning
MAT . *see* Magic-angle-turning
MCLR . *see* Multiconfigurational self-consistent field linear response theory
MCSCF . *see* Multiconfigurational self-consistent field
Membrane peptides and proteins **35** 1–84
Membranes **35** 2–3
Methanes, partial atomic charges **35** 91–4
Methyl carbon resonances **35** 352–3
Methyl effect **35** 99–100
Methyl group
  dynamics **35** 363–4, 383
  reorientation **35** 380–3
  spin-lattice relaxation **35** 383–5
  symmetry **35** 361–2
  thermodynamics **35** 364–5
  tunnelling **35** 365–6
Methyl thermometer **35** 383
Methyl tunnelling sidebands **35** 372–7
Methyl tunnelling spectroscopy **35** 366–77
Methylene carbon resonances **35** 352–3
Molecular dynamics **35** 332–3
Molecular internal dynamics **35** 314
Molecular motion **35** 49–51
Molecular orientational order **35** 215–7
Molecular tunnelling **35** 359–89
Møller-Plesset perturbation theory **35** 282–5
Mosaic spread **35** 11
Multiconfigurational self-consistent field linear response theory (MCLR) **35** 274–80
Multiconfigurational self-consistent field (MCSCF) **35** 274
Multipin crowns **35** 176

^{15}N NMR
  chemical shift tensors **35** 30–4
  chemical shifts **35** 34
  CSA **35** 13
  fd virus **35** 19–21
  gel-phase **35** 167
  gramicidin A **35** 29–34
  membranes **35** 4–5
  Pf1 **35** 21–2
^{15}N solid-state NMR, bacteriorhodopsin **35** 62
NMR tunnel resonance spectroscopy **35** 368–70
NOE . *see* Nuclear Overhauser effect
NOESY . *see* Nuclear Overhauser effect spectroscopy
Non-conjugated organic compounds, proton chemical shifts **35** 85–152
Norbornyl chlorides **35** 116
Nuclear Overhauser effect (NOE) pumping **35** 196–7
Nuclear Overhauser effect spectroscopy (NOESY)
  2D MAS **35** 172–3
  proteins **35** 17
Nuclear spin interactions **35** 207–11
Nuclear spin-spin coupling constants **35** 267–94

ODF . *see* Orientational distribution function
Off-resonance rf irradiation **35** 295–340
Olive oils **35** 341–57
On-resonance methods **35** 321
Ordered systems, 2D-PASS **35** 238–40
Organic compounds, atomic charges **35** 86
Orientation dependent spin interactions **35** 6–17
Orientational distribution function (ODF) **35** 216, 241–5
Oxygen substituent chemical shifts **35** 134–40

^{31}P NMR, gel-phase **35** 165–7
π pulses **35** 218–9
PASS . *see* Phase adjusted spinning sidebands
Peptide backbone **35** 26
  dihedral angles **35** 45–9
Peptide plane geometry **35** 39–45
Peptides, synthetic α-helical **35** 76–7
Perturbation theory
  linear response function **35** 285–7
  Møller-Plesset **35** 282–5
  Rayleigh-Schrödinger **35** 280–2
  time-dependent **35** 275–7
Pf1 **35** 21–2
PFG diffusion ordered NMR **35** 187–97
Phase adjusted spinning sidebands (PASS) **35** 207, 220, 237–50
Phonons **35** 383
PMR . *see* Proton magnetic resonance

Propagators **35** 217–21
see also Linear response function
Proton chemical shifts **35** 85–152
substituted methanes and ethanes **35** 91–4
Proton magnetic resonance (PMR) **35** 88
Proton shielding **35** 95–7, 150
Proton-decoupling **35** 205–6
Protons, steady-state magnetization **35** 331–2

Quadrupolar nuclei, 2D-PASS **35** 248–50

Rayleigh-Schrödinger perturbation theory **35** 280–2
REDOR . *see* Rotational echo double resonance
Reference frames **35** 211–3
Relaxation
see also Cross-relaxation
^{13}C **35** 156–8
fast exchange **35** 305–6
gramicidin A **35** 26
off-resonance rf irradiation **35** 297–306
rate calculation **35** 335–7
slow exchange **35** 306
Resins **35** 154–5
^{13}C chemical shifts **35** 155–6
^{13}C relaxation **35** 156–8
diffusion **35** 158–9
MAS **35** 158, 167–78
solvents **35** 167–9
Resolution, ^{1}H MAS NMR **35** 171–2
Retinal **35** 72
Retinal carbons **35** 62–3, 67
Rf-driven recoupling (RFDR) **35** 71–2, 75–6
Rf-field **35** 208–9
RFDR . *see* Rf-driven recoupling
Rhodopsin **35** 65–8
ROESY . *see* Rotating frame Overhauser spectroscopy
Rotating frame Overhauser spectroscopy (ROESY), off-resonance **35** 310–4
Rotational echo double resonance (REDOR) **35** 205
Rotational resonance **35** 71, 72–5, 205, 262

SAR . *see* Structure activity relationship
Schiff base **35** 62
SCS . *see* Substituent chemical shifts
SDS . *see* Sodium dodecyl sulfate
Second rank tensor interactions **35** 3
SEDRA . *see* Simple excitation for the dephasing of rotational-echo amplitudes
Self-relaxation rates **35** 302–3, 324–5
SELTICS . *see* Sideband eliminatio by temporay interruption of the chemical shift
Side chain orientation **35** 52–3
Sideband elimination by temporay interruption of the chemical shift (SELTICS) **35** 231–2
Sideband manipulation **35** 203–66
Simple excitation for the dephasing of rotational-echo amplitudes (SEDRA) **35** 71
Single bead analysis **35** 173–6
Slow exchange **35** 306, 318–9
Sodium dodecyl sulfate (SDS) micelles **35** 21
Solid phase synthesis **35** 154
Solid supports **35** 159–67
Solid-state ^{13}C NMR, retinal **35** 64
Solid-state ^{15}N NMR, retinal **35** 64
Solid-state NMR (SS NMR) **35** 205
membranes **35** 3
Solids **35** 205
Solution phase NMR **35** 178–85
Solvent-solute interaction **35** 319
Solvents, ^{1}H NMR **35** 167–8
Spectral density functions **35** 304–5
Spherical harmonics **35** 10
Spin-diffusion **35** 313–4
Spin-lattice relaxation, methyl group **35** 383–5
Spin-symmetry conversion **35** 379–80
Spin-symmetry species **35** 362–3
Spinning sidebands **35** 207, 215
SQUID . *see* Superconducting quantum interference device
SS NMR . *see* Solid-state NMR
Static solid-state NMR **35** 205
membrane peptides and proteins **35** 6–61
Steady-state magnetization **35** 329–34
Steric interactions **35** 94–9
Stromelysin **35** 185
Structural analysis
molecular motion **35** 49–51
multidimensional solid-state NMR **35** 79–80
Structure
bacteriorhodopsin **35** 62–5
gramicidin A **35** 25, 51–61
membrane peptides and proteins **35** 1–84
rhodopsin **35** 65–8
Structure activity relationship (SAR) by NMR **35** 185
Substituent chemical shifts (SCS) **35** 87, 88–9
bromine **35** 121–34
carbonyl **35** 140–9
chlorine **35** 116–21
fluorine **35** 109–16
halocyclohexanes **35** 127–30
iodine **35** 121–34
methyl **35** 99–100
oxygen **35** 134–40

Substituted methanes/ethanes, atomic charges **35** 91–4
Superconducting quantum interference device (SQUID)-detected NMR **35** 373–4
Synchronized MAS **35** 243
Synthetic α-helical peptides **35** 76–7

Tensor principal values **35** 29–30
Time-dependent perturbation theory **35** 275–7
TOCSY . *see* Total coherence spectroscopy
Torsion angles **35** 77–9, 210
TOSS . *see* Total suppression of spinning sidebands
Total coherence spectroscopy (TOCSY), proteins **35** 17
Total suppression of spinning sidebands (TOSS) **35** 207, 219, 221–36
Toxin α **35** 318
Transverse isotropy **35** 216
Tritium, tunnelling **35** 385–6
Tunnel resonance **35** 367
Tunnelling, isotope effects **35** 385–6
Tunnelling reservoir **35** 377–80

Unsaturated carbon resonance **35** 349

Vancomycin **35** 189

Wigner functions **35** 211–3

X-nucleus detection **35** 68

Zeeman interaction **35** 208–9

ELSEVIER

Progress in Nuclear Magnetic Resonance Spectroscopy

PROGRESS IN NUCLEAR
MAGNETIC RESONANCE
SPECTROSCOPY

www.elsevier.nl/locate/pnmrs

Contents of Previous Volumes

Volume 30
Intermolecular interactions characterized by nuclear Overhauser effects
H. Mo, T. C. Pochapsky
NMR diffusion measurements to characterise membrane transport and solute binding
A. R. Waldeck, P. W. Kuchel, A. J. Lennon, B. E. Chapman
Stray field magnetic resonance imaging
P. J. McDonald
Radiofrequency field gradient experiments
D. Canet
NMR techniques employing selective radiofrequency pulses in combination with pulsed field gradients
S. Berger
^{23}Na NMR methods for selective observation of sodium ions in ordered environments
R. Kemp-Harper, S. P. Brown, C. E. Hughes, P. Styles, S. Wimperis
Unravelling molecular structure and conformation—the modern role of coupling constants
W. A. Thomas
Toroids in NMR spectroscopy
J. W. Rathke, R. J. Klingler, R. E. Gerald II, K. W. Kramarz, K. Woelk
Book Review NMR Spectroscopy: Basic Principles, Concepts, and Applications in Chemistry, by H. Günther
– G. A. Morris

Volume 31
Radiofrequency microcoils in magnetic resonance
A. G. Webb
Magnetic resonance imaging of plants
J. A. Chudek, G. Hunter
Motional model analyses of protein and peptide dynamics using ^{13}C and ^{15}N NMR relaxation
V. A. Daragan, K. H. Mayo
Internet conferences in NMR spectroscopy
B. J. Hardy, S. W. Doughty, M. F. Parretti, J. Tennison, B. E. Finn, K. Gardner
Nuclear magnetic resonance spectroscopy of molecules in the gas phase
C. B. LeMaster
Quantitative localized ^{1}H MR spectroscopy for clinical use
R. Kreis
Reference deconvolution methods
G. A. Morris, H. Barjat, T. J. Horne
NMR studies of water bound to biological molecules
G. Otting
Erratum to "^{23}Na NMR methods for selective observation of sodium ions in ordered environments"
R. Kemp-Harper, S. P. Brown, C. E. Hughes, P. Styles, S. Wimperis
Parahydrogen induced polarization
Johannes Natterer, Joachim Bargon
Theory and calculation of nuclear shielding constants
H. Fukui
Characterizing porous media with NMR methods
A. Ted Watson, C. T. Philip Chang

Volume 32
Dipolar averaging in NMR spectroscopy: From polarization transfer to cross relaxation
R. Brüschweiler
Solid-state NMR investigations on the nature of hydrogen bonds
E. Brunner, U. Sternberg
Shaped radiofrequency pulses in high resolution NMR
R. Freeman
Ambiguous NOEs and automated NOE assignment
M. Nilges, S. I. O'Donoghue
Off-resonance nutation nuclear magnetic resonance spectroscopy of half-integer quadrupolar nuclei
A. P. M. Kentgens

Theories of chemical shift anisotropies in proteins and nucleic acids
D. SITKOFF, D. A. CASE
Technical aspects of NMR spectroscopy with biological macromolecules and studies of hydration in solution
GERHARD WIDER
NMR of large (> 25 kDa) proteins and protein complexes
CHERYL H. ARROWSMITH, YU-SUNG WU
The use of NMR methods for conformational studies of nucleic acids
S. S. WIJMENGA, B. N. M. VAN BUUREN

Volume 33
Pharmacokinetics using fluorine NMR in vivo
P. BACHERT
Quadrupole NMR relaxation of the noble gases dissolved in simple liquids and solutions. A critical review of experimental data in the light of computer simulation results
M. LUHMER, J. REISSE
A generalized ***k***-space formalism for treating the spatial aspects of a variety of NMR experiments
A. SODICKSON, D. G. CORY
NMR spectroscopy as a tool for structure-based drug design
B.J. STOCKMAN
^{13}C NMR spectroscopy of monoterpenoids
M. J. P. FERREIRA, V. P. EMERENCIANO, G. A. R. LINIA, P. ROMOFF, P. A. T. MACARI, G. V. RODRIGUES
Protein NMR relaxation: theory, applications and outlook
M. W. F. FISCHER, A. MAJUMDAR, E. R. P. ZUIDERWEG
NMR imaging of materials
J. B. MILLER

Volume 34
Application of Lie algebra to NMR spectroscopy
J. H. KRISTENSEN, H. BILDSØE, H. J. JAKOBSEN, N. C. NIELSEN
Applications of the parahydrogen phenomenon: A chemical perspective
S. B. DUCKETT, C. J. SLEIGH
Heteronuclear multidimensional NMR experiments for the structure determination of proteins in solution employing pulsed field gradients
M. SATTLER, J. SCHLEUCHER, C. GRIESINGER
Recent advances in experimental solid state NMR methodology for half-integer spin quadrupolar nuclei
M. E. SMITH, E. H. R. VAN ECK
Diffusion ordered nuclear magnetic resonance spectroscopy: principles and applications
C. S. JOHNSON JR.
Linear prediction spectral analysis of NMR data
P. KOEHL
Cerebral amino acids studied by nuclear magnetic resonance spectroscopy in vivo
S. WILLIAMS
Nuclear magnetic resonance studies of crown ethers
G. W. BUCHANAN

Volume 35
Static and magic angle spinning NMR of membrane peptides and proteins
J. H. DAVIS AND M. AUGER
A model for the calculation of proton chemical shifts in non-conjugated organic compounds
RAYMOND J. ABRAHAM
NMR methods utilized in combinatorial chemistry research
M. J. SHAPIRO AND J. S. GOUNARIDES
Sideband manipulation in magic-angle-spinning nuclear magnetic resonance
O. N. ANTZUTKIN
Theory and calculation of nuclear spin–spin coupling constants
H. FUKUI
Study of dynamic processes in liquids using off-resonance rf irradiation
H. DESVAUX AND P. BERTHAULT
Application of NMR to the study of olive oils
G. VLAHOV
Quantum tunnelling aspects of methyl group rotation studied by NMR
A. J. HORSEWILL